

chain nodes :

7 20

ring nodes :

1 2 3 4 5 6 8 9 10 11 12 13 14 15 16

chain bonds :

6-7 7-8 9-20

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 8-9 8-12 9-10 10-11 11-12 11-13 12-16 13-14 14-15
15-16

exact/norm bonds :

1-2 1-6 2-3 3-4 4-5 5-6 8-9 8-12 9-20

exact bonds :

6-7 7-8 9-10 10-11

normalized bonds :

11-12 11-13 12-16 13-14 14-15 15-16

isolated ring systems :

containing 1 : 8 :

G1:0,S

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:Atom 9:Atom 10:Atom 11:Atom
12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 20:CLASS

* * * * * * * * * * Welcome to STN International * * * * * * * * *

| | |
|-----------------------|--|
| <u>NEWS 1</u> | Web Page URLs for STN Seminar Schedule - N. America |
| <u>NEWS 2</u> | "Ask CAS" for self-help around the clock |
| <u>NEWS 3</u> NOV 24 | MSDS-CCOHS file reloaded |
| <u>NEWS 4</u> DEC 08 | CABA reloaded with left truncation |
| <u>NEWS 5</u> DEC 08 | IMS file names changed |
| <u>NEWS 6</u> DEC 17 | DGENE: Two new display fields added |
| <u>NEWS 7</u> DEC 18 | BIOTECHNO no longer updated |
| <u>NEWS 8</u> DEC 19 | CROPUS no longer updated; subscriber discount no longer available |
| <u>NEWS 9</u> DEC 22 | ABI-INFORM now available on STN |
| <u>NEWS 10</u> JAN 27 | Source of Registration (SR) information in REGISTRY updated and searchable |
| <u>NEWS 11</u> JAN 27 | A new search aid, the Company Name Thesaurus, available in CA/CAplus |
| <u>NEWS 12</u> FEB 05 | German (DE) application and patent publication number format changes |
| <u>NEWS 13</u> MAR 03 | MEDLINE and LMEDLINE reloaded |
| <u>NEWS 14</u> MAR 03 | MEDLINE file segment of TOXCENTER reloaded |
| <u>NEWS 15</u> MAR 03 | FRANCEPAT now available on STN |
| <u>NEWS 16</u> MAR 29 | Pharmaceutical Substances (PS) now available on STN |
| <u>NEWS 17</u> MAR 29 | WPIFV now available on STN |
| <u>NEWS 18</u> MAR 29 | No connect hour charges in WPIFV until May 1, 2004 |
| <u>NEWS 19</u> MAR 29 | New monthly current-awareness alert (SDI) frequency in RAPRA |

| | |
|---------------------|---|
| <u>NEWS EXPRESS</u> | MARCH 31 CURRENT WINDOWS VERSION IS V7.00A, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 3 MARCH 2004 |
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| <u>NEWS INTER</u> | General Internet Information |
| <u>NEWS LOGIN</u> | Welcome Banner and News Items |
| <u>NEWS PHONE</u> | Direct Dial and Telecommunication Network Access to STN |
| <u>NEWS WWW</u> | CAS World Wide Web Site (general information) |

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| COST IN U.S. DOLLARS | SINCE FILE ENTRY | TOTAL SESSION |
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| FULL ESTIMATED COST | 0.21 | 0.21 |

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STRUCTURE FILE UPDATES: 7 APR 2004 HIGHEST RN 672883-15-7
 DICTIONARY FILE UPDATES: 7 APR 2004 HIGHEST RN 672883-15-7

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

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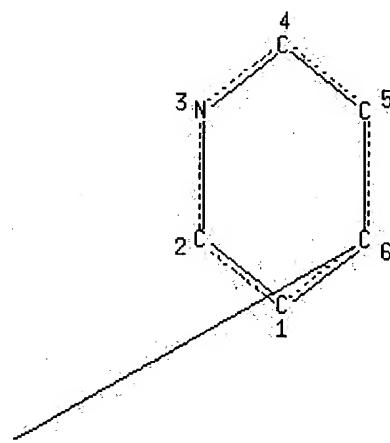
Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:
<http://www.cas.org/ONLINE/DBSS/registryss.html>

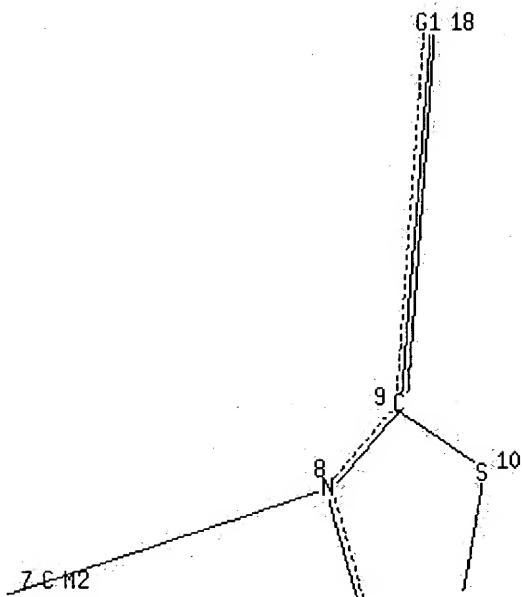
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=> l1
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 The previous command name entered was not recognized by the system.
 For a list of commands available to you in the current file, enter "HELP COMMANDS" at an arrow prompt (>):

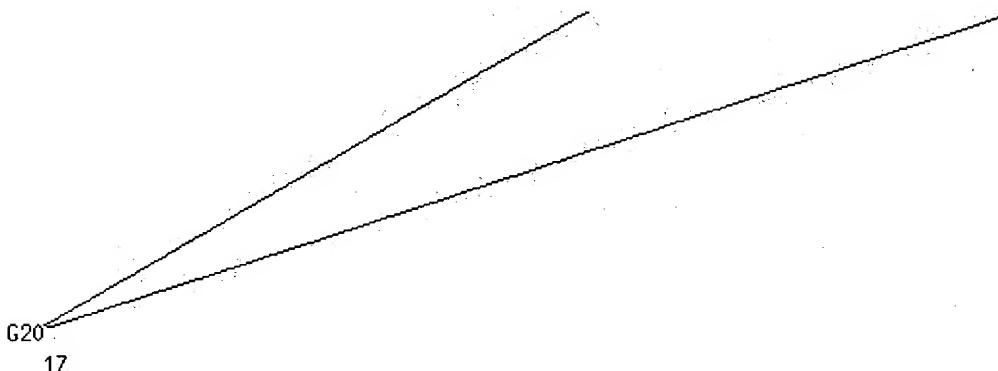
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 0 19 S 20



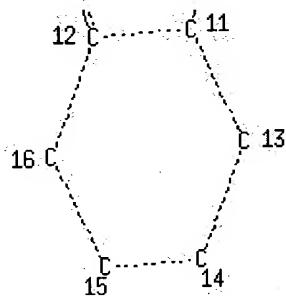
Page 1-A



Page 1-B



Page 2-A



Page 2-B

VAR G1=19/20

REP G20=(1-2) 7-6 7-8

NODE ATTRIBUTES:

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| NSPEC | IS R | AT | 1 |
| NSPEC | IS R | AT | 2 |
| NSPEC | IS R | AT | 3 |
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| NSPEC | IS R | AT | 5 |
| NSPEC | IS R | AT | 6 |
| NSPEC | IS C | AT | 7 |
| NSPEC | IS R | AT | 8 |
| NSPEC | IS R | AT | 9 |

NSPEC IS R AT 10
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 NSPEC IS R AT 12
 NSPEC IS R AT 13
 NSPEC IS R AT 14
 NSPEC IS R AT 15
 NSPEC IS R AT 16
 NSPEC IS C AT 17
 NSPEC IS C AT 18
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 MLEVEL IS CLASS AT 7 19 20
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RSPEC I
 NUMBER OF NODES IS 20

STEREO ATTRIBUTES: NONE

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 SAMPLE SCREEN SEARCH COMPLETED - 5 TO ITERATE

100.0% PROCESSED 5 ITERATIONS 2 ANSWERS
 SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
 BATCH **COMPLETE**
 PROJECTED ITERATIONS: 5 TO 234
 PROJECTED ANSWERS: 2 TO 124

L2 2 SEA SSS SAM L1

=> s 11 full
 THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 155.00 U.S. DOLLARS
 DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
 FULL SEARCH INITIATED 15:25:36 FILE 'REGISTRY'
 FULL SCREEN SEARCH COMPLETED - 104 TO ITERATE

100.0% PROCESSED 104 ITERATIONS 45 ANSWERS
 SEARCH TIME: 00.00.01

L3 45 SEA SSS FUL L1

=> file hcplus
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 ENTRY SESSION
 FULL ESTIMATED COST 157.10 157.31

FILE 'HCPLUS' ENTERED AT 15:25:39 ON 09 APR 2004
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FILE COVERS 1907 - 9 Apr 2004 VOL 140 ISS 16
FILE LAST UPDATED: 8 Apr 2004 (20040408/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

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L4 7 L3

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69 ROCHER, J?/AU
L5 1 L4 AND ROCHER, J?/AU

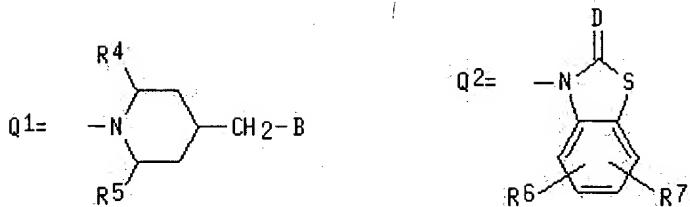
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L5 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2004 ACS on STN

| Full Text | Citing References |
|-------------------------|--|
| ACCESSION NUMBER: | 1999:311193 HCAPLUS |
| DOCUMENT NUMBER: | 130:338102 |
| TITLE: | Preparation of N-(aminoalkyl)- or N-(1-piperidinylmethyl)benzothiazoline derivatives as ligands for sigma-receptor |
| INVENTOR(S): | Rocher, Jean-Philippe; Yamabe, Haruko; Chaki, Haruyuki; Saito, Ken-ichi; Abe, Michikazu; Okuyama, Masahiro |
| PATENT ASSIGNEE(S): | Mitsubishi Chemical Corporation, Japan |
| SOURCE: | PCT Int. Appl., 95 pp.
CODEN: PIXXD2 |
| DOCUMENT TYPE: | Patent |
| LANGUAGE: | Japanese |
| FAMILY ACC. NUM. COUNT: | 1 |

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|--|-------------------|----------|-----------------|------------|
| WO 9923083 | A1 | 19990514 | WO 1998-JP4973 | 19981104 |
| W: CA, CN, KR, US | | | | |
| RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE | | | | |
| EP 1043319 | A1 | 20001011 | EP 1998-951687 | 19981104 |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI | | | | |
| JP 11217377 | A2 | 19990810 | JP 1998-314459 | 19981105 |
| PRIORITY APPLN. INFO.: | | | JP 1997-302607 | A 19971105 |
| | | | WO 1998-JP4973 | W 19981104 |
| OTHER SOURCE(S): | MARPAT 130:338102 | | | |
| GI | | | | |



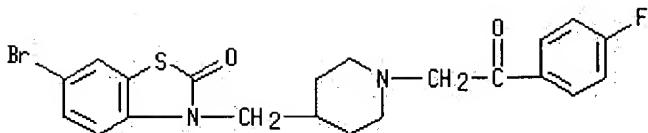
AB Compds. represented by the following formula, such as (R,S)-1-(1-adamantyl)-2-[4-(6-chloro-2-iminobenzothiazolin-3-ylmethyl)piperidin-1-yl]ethanol, or salts thereof: X-Q-C(R1)(R2)-Z [wherein R1 and R2 each represents hydrogen, alkyl, cycloalkyl, hydroxyalkyl, or alkenyl; and Z represents either of groups NR₃(CH₂)_p and Q1; wherein R₃ represents alkyl, cycloalkyl, hydroxyalkyl, or alkenyl; p is an integer of 3 to 8; R₄ and R₅ each represents hydrogen or alkyl or they together with other interposing atoms represent a 5- to 7-membered heterocyclic ring; and B represents formula Q2 (wherein R₆ and R₇ each represents hydrogen, halogeno, NO₂, alkyl, cycloalkyl, alkenyl, haloalkyl, OH, alkoxy, haloalkoxy, alkoxy carbonyl, Ph, (un)substituted NH₂, alkylthio, etc.); D represents sulfur, oxygen, or (un)substituted NH; when X represents optionally alkyl-substituted mono- or polycyclic alkyl, cycloalkylalkyl, aryl, or heteroaryl, Q represents CO, C(:NOH), C(Y)(A) (wherein Y represents H, alkyl, alkenyl, alkynyl, etc. and A represent OH, alkoxy, cycloalkoxy, cycloalkylalkoxy, alkenyloxy, aryloxy, etc.); or when X represents a 8- to 10-membered bicyclic heteroaryl contg. 1 or 2 heteroatoms, Q represents single bond], which have high affinity to σ -receptors and exhibit small inhibition consts. Ki against σ -1 and/or σ -2 receptors, are prep'd. Also claimed are therapeutics contg. I as the active ingredients for the treatment and/or prevention of diseases caused or enhanced by nerve-regulating effect of σ -ligands. They are useful for the treatment and/or prevention of central nervous system diseases, intestinal diseases, and cardiovascular diseases. Thus, 4-(6-chloro-2-iminobenzothiazolin-3-ylmethyl)piperidine was condensed with 1-(bromoacetyl)adamantane in the presence of K₂CO₃ followed by NaBH₄ redn. in ethanol and THF and acidification with HCl in EtOAc to give 1-(1-adamantyl)-2-[4-(6-chloro-2-iminobenzothiazolin-3-ylmethyl)piperidin-1-yl]ethanol hydrochloride (II). II and 3-[[1-[2-(4-fluorophenyl)-2-oxoethyl]-4-piperidinyl]methyl]-5-chloro-2-oxobenzothiazoline hydrochloride inhibited the binding of [³H]-di-o-tolylguanidine to σ -receptor (P2 membrane fraction) prep'n. from rat liver with Ki value of 7.0 and 3.1 nM, resp., as compared to Ki of 29 nM for haloperidol. A tablet, an injection, and an ointment formulation contg. II were described.

IT 224443-05-4P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prep'n. of N-(aminoalkyl)- or N-(1-piperidinyl)benzothiazoline derivs. having high affinity to sigma-receptor as therapeutics)

RN 224443-05-4 HCPLUS

CN 2(3H)-Benzothiazolone, 6-bromo-3-[[1-[2-(4-fluorophenyl)-2-oxoethyl]-4-piperidinyl]methyl]-, monohydrochloride (9CI) (CA INDEX NAME)



HCl

REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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(FILE 'HOME' ENTERED AT 15:22:35 ON 09 APR 2004)

FILE 'REGISTRY' ENTERED AT 15:22:40 ON 09 APR 2004

L1 STRUCTURE uploaded
L2 2 S L1
L3 45 S L1 FULL

FILE 'HCAPLUS' ENTERED AT 15:25:39 ON 09 APR 2004

L4 7 S L3
L5 1 S L4 AND ROCHER, J?/AU

=> s 14 and yamabe, h?/au

208 YAMABE, H?/AU

L6 1 L4 AND YAMABE, H?/AU

=> s 16 not 15

L7 0 L6 NOT L5

=> s 14 and chaki, h?/au

74 CHAKI, H?/AU

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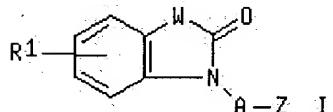
L4 ANSWER 1 OF 7 HCAPLUS COPYRIGHT 2004 ACS on STN

| | |
|------|------------|
| Full | Citing |
| Text | References |

ACCESSION NUMBER: 2001:372159 HCAPLUS

DOCUMENT NUMBER: 134:366868
 TITLE: Preparation of benzothiazolines as neuropeptide Y receptor antagonists
 INVENTOR(S): Sato, Yoshiya; Itani, Hiromichi; Tabuchi, Seiichiro;
 Sakata, Yoshihiko; Ohashi, Hiroko
 PATENT ASSIGNEE(S): Fujisawa Pharmaceutical Co., Ltd., Japan
 SOURCE: Jpn. Kokai Tokkyo Koho, 88 pp.
 CODEN: JKXXAF
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|-------------------------------|-------------------|----------|-----------------------|------------|
| <u>JP 2001139574</u> | A2 | 20010522 | <u>JP 2000-296175</u> | 20000928 |
| <u>PRIORITY APPLN. INFO.:</u> | | | <u>AU 1999-3093</u> | A 19990928 |
| OTHER SOURCE(S): | MARPAT 134:366868 | | | |
| GI | | | | |



AB The title compds. I [R1 = H, halo; W = S, O; A = (CH₂)_n, etc.; n = 1 - 6; Z = (un)substituted N-contg. heterocyclic ring] are prep'd. 1-[(5-Chloro-2-oxobenzothiazolin-3-yl)acetyl]piperidine-4-carboxylic acid 4-benzoylanilide showed IC100 of 10⁻⁷ M in a neuropeptide Y5 receptor binding assay.

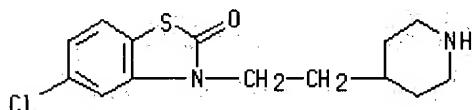
IT 340179-40-0P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(prepn. of benzothiazolines as neuropeptide Y receptor antagonists)

RN 340179-40-0 HCPLUS

CN 2(3H)-Benzothiazolone, 5-chloro-3-[2-(4-piperidinyl)ethyl]- (9CI) (CA INDEX NAME)



L4 ANSWER 2 OF 7 HCPLUS COPYRIGHT 2004 ACS on STN

| | |
|-----------|-------------------|
| Full Text | Citing References |
|-----------|-------------------|

ACCESSION NUMBER: 1999:311193 HCPLUS
 DOCUMENT NUMBER: 130:338102
 TITLE: Preparation of N-(aminoalkyl)- or N-(1-piperidinylmethyl)benzothiazoline derivatives as ligands for sigma-receptor
 INVENTOR(S): Rocher, Jean-Philippe; Yamabe, Haruko; Chaki, Haruyuki; Saito, Ken-ichi; Abe, Michikazu; Okuyama, Masahiro
 PATENT ASSIGNEE(S): Mitsubishi Chemical Corporation, Japan

SOURCE: PCT Int. Appl., 95 pp.

CODEN: PIXXD2

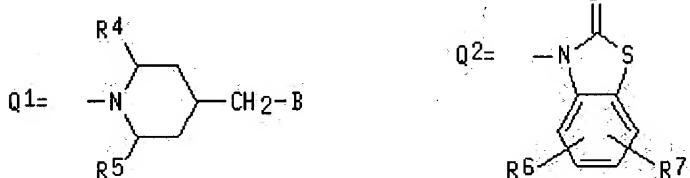
DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

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| <u>WO 9923083</u> | A1 | 19990514 | <u>WO 1998-JP4973</u> | 19981104 |
| W: CA, CN, KR, US
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE | | | | |
| <u>EP 1043319</u> | A1 | 20001011 | <u>EP 1998-951687</u> | 19981104 |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI | | | | |
| <u>JP 11217377</u> | A2 | 19990810 | <u>JP 1998-314459</u> | 19981105 |
| <u>PRIORITY APPLN. INFO.:</u> | | | <u>JP 1997-302607</u> | A 19971105 |
| | | | <u>WO 1998-JP4973</u> | W 19981104 |
| OTHER SOURCE(S): MARPAT 130:338102 | | | | |
| GI | | | | |



AB Compds. represented by the following formula, such as (R,S)-1-(1-adamantyl)-2-[4-(6-chloro-2-iminobenzothiazolin-3-ylmethyl)piperidin-1-yl]ethanol, or salts thereof: X-Q-C(R1)(R2)-Z [wherein R1 and R2 each represents hydrogen, alkyl, cycloalkyl, hydroxyalkyl, or alkenyl; and Z represents either of groups NR3(CH2)p and Q1; wherein R3 represents alkyl, cycloalkyl, hydroxyalkyl, or alkenyl; p is an integer of 3 to 8; R4 and R5 each represents hydrogen or alkyl or they together with other interposing atoms represent a 5- to 7-membered heterocyclic ring; and B represents formula Q2 (wherein R6 and R7 each represents hydrogen, halogeno, NO2, alkyl, cycloalkyl, alkenyl, haloalkyl, OH, alkoxy, haloalkoxy, alkoxycarbonyl, Ph, (un)substituted NH2, alkylthio, etc.); D represents sulfur, oxygen, or (un)substituted NH; when X represents optionally alkyl-substituted mono- or polycyclic alkyl, cycloalkylalkyl, aryl, or heteroaryl, Q represents CO, C(:NOH), C(Y)(A) (wherein Y represents H, alkyl, alkenyl, alkynyl, etc. and A represent OH, alkoxy, cycloalkoxy, cycloalkylalkoxy, alkenyloxy, aryloxy, etc.); or when X represents a 8- to 10-membered bicyclic heteroaryl contg. 1 or 2 heteroatoms, Q represents single bond], which have high affinity to σ -receptors and exhibit small inhibition consts. Ki against σ -1 and/or σ -2 receptors, are prep'd. Also claimed are therapeutics contg. I as the active ingredients for the treatment and/or prevention of diseases caused or enhanced by nerve-regulating effect of σ -ligands. They are useful for the treatment and/or prevention of central nervous system diseases, intestinal diseases, and cardiovascular diseases. Thus, 4-(6-chloro-2-iminobenzothiazolin-3-ylmethyl)piperidine was condensed with 1-(bromoacetyl)adamantane in the presence of K2CO3 followed by NaBH4 redn. in ethanol and THF and acidification with HCl in EtOAc to give 1-(1-adamantyl)-2-[4-(6-chloro-2-iminobenzothiazolin-3-ylmethyl)piperidin-

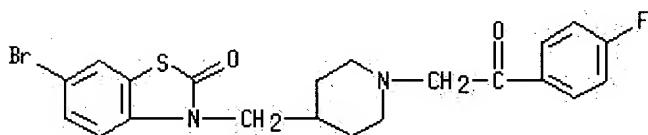
1-yl]ethanol hydrochloride (II). II and 3-[[1-[2-(4-fluorophenyl)-2-oxoethyl]-4-piperidinyl]methyl]-5-chloro-2-oxobenzothiazoline hydrochloride inhibited the binding of [³H]-di-o-tolylguanidine to σ-receptor (P2 membrane fraction) prepn. from rat liver with Ki value of 7.0 and 3.1 nM, resp., as compared to Ki of 29 nM for haloperidol. A tablet, an injection, and an ointment formulation contg. II were described.

IT 224443-05-4P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of N-(aminoalkyl)- or N-(1-piperidinyl)benzothiazoline derivs. having high affinity to sigma-receptor as therapeutics)

RN 224443-05-4 HCAPLUS

CN 2(3H)-Benzothiazolone, 6-bromo-3-[[1-[2-(4-fluorophenyl)-2-oxoethyl]-4-piperidinyl]methyl]-, monohydrochloride (9CI) (CA INDEX NAME)



HCl

REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 3 OF 7 HCAPLUS COPYRIGHT 2004 ACS on STN

 Full Text Citing References

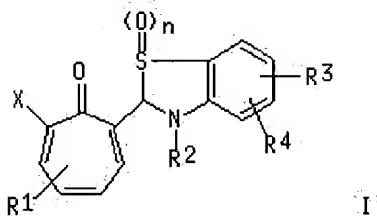
ACCESSION NUMBER: 1993:191730 HCAPLUS
 DOCUMENT NUMBER: 118:191730
 TITLE: Preparation of benzothiazolinyltropolones for treatment of ischemia.
 INVENTOR(S): McWhoster, William W.; Ito, Norie; Ozawa, Kazunori; Kushida, Hiroshi; Nomura, Toshiharu; Kunihara, Mineo
 PATENT ASSIGNEE(S): Upjohn Co., USA
 SOURCE: Jpn. Kokai Tokkyo Koho, 14 pp.
 CODEN: JKXXAF
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 3

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|------|----------|-----------------|----------|
| JP 04247077 | A2 | 19920903 | JP 1991-56252 | 19910131 |
| CA 2087004 | AA | 19920301 | CA 1991-2087004 | 19910827 |
| CA 2087004 | C | 19980421 | | |
| EP 546102 | A1 | 19930616 | EP 1991-917948 | 19910827 |
| EP 546102 | B1 | 19971015 | | |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE | | | | |
| HU 65943 | A2 | 19940829 | HU 1993-533 | 19910827 |
| JP 06509318 | T2 | 19941020 | JP 1991-516629 | 19910827 |
| JP 2512656 | B2 | 19960703 | | |
| AT 159251 | E | 19971115 | AT 1991-917948 | 19910827 |
| ES 2109276 | T3 | 19980116 | ES 1991-917948 | 19910827 |

| | | | | |
|-------------------------------|---|----------|-----------------------|----------|
| <u>NO 9300669</u> | A | 19930225 | <u>NO 1993-669</u> | 19930225 |
| <u>US 5594144</u> | A | 19970114 | <u>US 1995-442710</u> | 19950518 |
| <u>US 5703071</u> | A | 19971230 | <u>US 1995-443972</u> | 19950518 |
| <u>PRIORITY APPLN. INFO.:</u> | | | <u>JP 1990-229536</u> | 19900829 |
| | | | <u>JP 1991-56252</u> | 19910131 |
| | | | <u>JP 1991-39173</u> | 19910208 |
| | | | <u>WO 1991-US5906</u> | 19910827 |
| | | | <u>US 1993-975924</u> | 19930218 |

OTHER SOURCE(S) : MARPAT 118:191730
GI



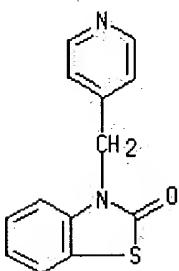
AB The title compds. [I; R1 = H, alkyl, (un)substituted aryl; R2 = H, alkyl, etc.; R3, R4 = H, alkyl, halo, OH, alkoxy, etc.; X = OH, alkoxy, etc.; n = 0, 1, 2] were prep'd. E.g., 2-[(2-phenylethyl)amino]thiophenol (prepn. given) was refluxed with 2-methoxy-4-isopropyl-7-formyl-2,4,6-cycloheptatrien-1-one in toluene for 17 H to give I [X = MeO, R1 = 5'-iso-Pr, R2 = PhCH2CH2, R3 = R4 = H, n = 0]. At 0.1 mg/Kg i.p. this showed 50% effectiveness in counteracting brain ischemic rats in a learning study using rats.

IT **142224-26-8P**

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of, as intermediate for benzothiazolinyltropolones for treatment of ischemia)

RN 142224-26-8 HCAPLUS

CN 2(3H)-Benzothiazolone, 3-(4-pyridinylmethyl)- (9CI) (CA INDEX NAME)



L4 ANSWER 4 OF 7 HCAPLUS COPYRIGHT 2004 ACS on STN

| | |
|-----------|-------------------|
| Full Text | Citing References |
|-----------|-------------------|

ACCESSION NUMBER:

1992:531223 HCAPLUS

DOCUMENT NUMBER:

117:131223

TITLE:

Preparation of heterocycltropolones as ischemia inhibitors

INVENTOR(S) :

Ito, Norie; Kunihara, Mineo; Kushida, Hiroshi;
McWhoster, William W.; Nomura, Syunji; Ozawa,
Kazunori; Taniguchi, Mikeo; Tsuzuki, Tazuo

PATENT ASSIGNEE(S) :

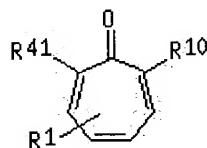
USA

SOURCE: PCT Int. Appl., 77 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

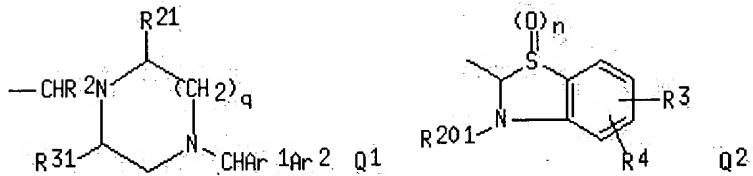
| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|------|----------|-----------------------|----------|
| <u>WO 9204338</u> | A1 | 19920319 | <u>WO 1991-US5906</u> | 19910827 |
| W: AU, BB, BG, BR, CA, CS, FI, HU, JP, KP, KR, LK, MC, MG, MN, MW,
NO, PL, RO, SD, SU, US | | | | |
| RW: AT, BE, BJ, CF, CG, CH, CI, CM, DE, DK, ES, FR, GA, GB, GN, GR,
IT, LU, ML, MR, NL, SE, SN | | | | |
| <u>JP 04120069</u> | A2 | 19920421 | <u>JP 1990-229536</u> | 19900829 |
| <u>AU 9187203</u> | A1 | 19920330 | <u>AU 1991-87203</u> | 19910827 |
| <u>AU 651629</u> | B2 | 19940728 | | |
| <u>EP 546102</u> | A1 | 19930616 | <u>EP 1991-917948</u> | 19910827 |
| <u>EP 546102</u> | B1 | 19971015 | | |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE | | | | |
| <u>HU 65943</u> | A2 | 19940829 | <u>HU 1993-533</u> | 19910827 |
| <u>JP 06509318</u> | T2 | 19941020 | <u>JP 1991-516629</u> | 19910827 |
| <u>JP 2512656</u> | B2 | 19960703 | | |
| <u>NO 9300669</u> | A | 19930225 | <u>NO 1993-669</u> | 19930225 |
| <u>PRIORITY APPLN. INFO.:</u> | | | <u>JP 1990-229536</u> | 19900829 |
| | | | <u>JP 1991-56252</u> | 19910131 |
| | | | <u>JP 1991-39173</u> | 19910208 |
| | | | <u>WO 1991-US5906</u> | 19910827 |

OTHER SOURCE(S) : MARPAT 117:131223

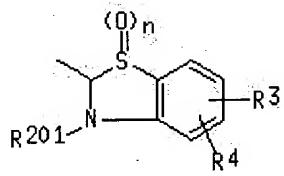
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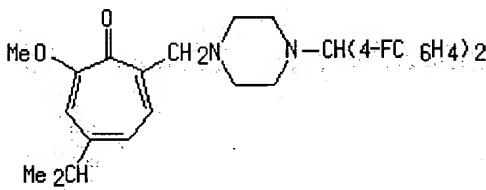
I



II



III



IV

AB Title compds. I [R10 = Q1, Q2; R1, R2 = H, C1-5 alkyl, (substituted) aryl, (substituted) heterocycl; R3, R4 = H, (substituted) C1-5 alkyl, C7-20 aralkyl, C7-20 aralkyl contg. O, S, or N atoms; halo, OH, C1-5 alkoxy, cyano, etc.; R41 = OR3, OR6, NR7R8, etc.; R6 = H, (substituted) C1-5 alkyl, etc.; R7, R8 = H, (substituted) C1-5 alkyl, C7-20 aralkyl which may contain O, S, or N atoms; NR7R8 = 5-7 membered ring which may contain

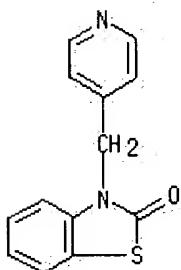
addnl. O or N atoms; R21, R31 = H, C1-3 alkyl; R201 = H, C1-5 alkyl, C2-20 aralkyl, C6-10 arylsulfonyl, C6-10 arylsulfonyl contg. O, S, or N atoms; Ar1, Ar2 = (substituted) aryl; n = 0-2; q = 1-2], were prep'd. Thus, a soln. of 7-chloromethyl-4-isopropyl-2-methoxy-4-isopropyl-2,4,6-cycloheptatrien-1-one (prepn. given), 1-(4,4'-difluorobenzhydryl)piperazine, and Et3N in CHCl₃ was refluxed for 20 h to give title compd. II. II had minimal ED of <5 mg/kg i.v. in a ischemic heart/reperfusion test in rats.

IT 142224-26-8P

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of, as intermediate for ischemia inhibitors)

RN 142224-26-8 HCPLUS

CN 2(3H)-Benzothiazolone, 3-(4-pyridinylmethyl)- (9CI) (CA INDEX NAME)



L4 ANSWER 5 OF 7 HCPLUS COPYRIGHT 2004 ACS on STN

| | |
|-----------|-------------------|
| Full Text | Citing References |
|-----------|-------------------|

ACCESSION NUMBER:

1987:84351 HCPLUS

DOCUMENT NUMBER:

106:84351

TITLE:

2-(4-Pyridyl)ethyl as a protective group for sulfur functionality

AUTHOR(S):

Katritzky, Alan R.; Takahashi, Ichiro; Marson, Charles M.

CORPORATE SOURCE:

Dep. Chem., Univ. Florida, Gainesville, FL, 32611, USA

SOURCE:

Journal of Organic Chemistry (1986), 51(25), 4914-20

CODEN: JOCEAH; ISSN: 0022-3263

DOCUMENT TYPE:

Journal

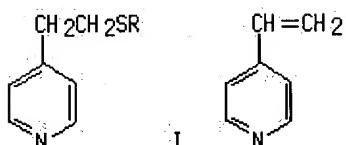
LANGUAGE:

English

OTHER SOURCE(S):

CASREACT 106:84351

GI



AB 2-(4-Pyridyl)ethyl sulfides I (R = octyl, 2-naphthyl, Ph) were prep'd. by Michael addn. of 4-vinylpyridine (II) with thiols RSH, whereas I [R = 5-nitro-2-pyridyl, CH₂Ph, Bu, Bz, (Phs)CO] were prep'd. by alkylation of thiol I (R = H) with RX (X = halide). I (R = CH₂Ph) was also prep'd. by alkylation of PhCH₂SH with halide I (R = Cl). These sulfides and their corresponding sulfoxides and sulfones were depyridylethylated by quaternization and subsequent treatment with mild base to give the corresponding thiols, sulfinic acids, sulfonic acids, and sulfenamides. During one of these protection-deprotection sequences, Me 1-octyl sulfoxide was readily converted by aerial oxidn. into the corresponding

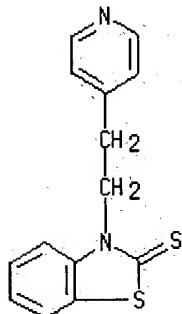
sulfone.

IT 27410-87-3

RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with vinylpyridine)

RN 27410-87-3 HCAPLUS

CN 2(3H)-Benzothiazolethione, 3-[2-(4-pyridinyl)ethyl]- (9CI) (CA INDEX
NAME)



L4 ANSWER 6 OF 7 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text Citing References

ACCESSION NUMBER: 1971:87880 HCAPLUS
 DOCUMENT NUMBER: 74:87880
 TITLE: Michael and Mannich reactions with
benzothiazole-2-thiol
 AUTHOR(S): Halasa, Adel F.; Smith, George E. P., Jr.
 CORPORATE SOURCE: Cent. Res. Lab., Firestone Tire and Rubber Co., Akron,
OH, USA
 SOURCE: Journal of Organic Chemistry (1971), 36(5), 636-41
 CODEN: JOCEAH; ISSN: 0022-3263

DOCUMENT TYPE: Journal
 LANGUAGE: English

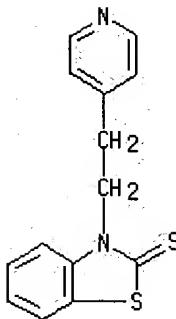
AB The reaction of the anion of benzothiazole-2-thiol (MBT) with activated olefins in the presence of NaH with Michael reaction acceptors produced 3-substituted benzothiazoline-2-thiones. Similarly, the Mannich reaction of MBT anion with HCHO and primary or secondary amines produced the N- (or 3-) substituted benzothiazoline-2-thiones. Possible mechanisms and supporting NMR, ir, and uv data are discussed. The N substitution of MBT anion is discussed within the framework of the oxibase scale which can predict the condition for formation of N products or S products from this ambident anion.

IT 27410-87-3P

RL: SPN (Synthetic preparation); PREP (Preparation)
(prep. of)

RN 27410-87-3 HCAPLUS

CN 2(3H)-Benzothiazolethione, 3-[2-(4-pyridinyl)ethyl]- (9CI) (CA INDEX
NAME)



L4 ANSWER 7 OF 7 HCAPLUS COPYRIGHT 2004 ACS on STN

| | |
|-----------|-------------------|
| Full Text | Citing References |
|-----------|-------------------|

ACCESSION NUMBER: 1971:53769 HCAPLUS
 DOCUMENT NUMBER: 74:53769
 TITLE: 3-Substituted-2-benzothiazolinethiones
 INVENTOR(S): Halasa, Adel F.
 PATENT ASSIGNEE(S): Firestone Tire and Rubber Co.
 SOURCE: U.S., 3 pp.
 CODEN: USXXAM
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------------------------|------|----------|-----------------|----------|
| US 3538109 | A | 19701103 | US 1967-655761 | 19670725 |
| PRIORITY APPLN. INFO.: | | | US 1967-655761 | 19670725 |

GI For diagram(s), see printed CA Issue.

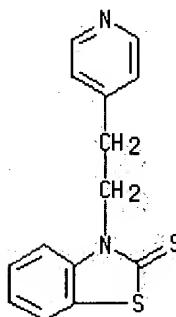
AB The title compds. (I) are all delayed-action rubber accelerators produced by Michael addns. to benzothiazoline-2-thione (II). Thus, II in freshly distd. THF stirred 48 hr with 4-vinylpyridine and NaH gave I (X = H, Y = 4-pyridyl), m. 159-61°. The corresponding I (X = H, Y = 2-pyridyl), m. 94-5° (alc.), was produced similarly. Analogous reaction of EtCH(NO₂)CH₂OAc with II give I (X = NO₂, Y = Et), m. 89-90°. Similar Michael condensation of BzCH₂CH₂Cl with II yielded I (X = H, Y = Bz), m. 144.5-5.0° (CHCl₃-EtOH).

IT 27410-87-3P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (prep. of)

RN 27410-87-3 HCAPLUS

CN 2(3H)-Benzothiazolethione, 3-[2-(4-pyridinyl)ethyl]- (9CI) (CA INDEX NAME)



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| => file caold | | | |
| COST IN U.S. DOLLARS | SINCE FILE ENTRY | TOTAL SESSION | |
| FULL ESTIMATED COST | 45.13 | 202.44 | |
| DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) | SINCE FILE ENTRY | TOTAL SESSION | |
| CA SUBSCRIBER PRICE | -5.54 | -5.54 | |

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FILE COVERS 1907-1966
 FILE LAST UPDATED: 01 May 1997 (19970501/UP)

This file contains CAS Registry Numbers for easy and accurate substance identification. Title keywords, authors, patent assignees, and patent information, e.g., patent numbers, are now searchable from 1907-1966. TIFF images of CA abstracts printed between 1907-1966 are available in the PAGE display formats.

This file supports REGISTRY for direct browsing and searching of all substance data from the REGISTRY file. Enter HELP FIRST for more information.

=> d his

(FILE 'HOME' ENTERED AT 15:22:35 ON 09 APR 2004)

FILE 'REGISTRY' ENTERED AT 15:22:40 ON 09 APR 2004

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| L2 | 2 S L1 |
| L3 | 45 S L1 FULL |

FILE 'HCAPLUS' ENTERED AT 15:25:39 ON 09 APR 2004

| | |
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| L4 | 7 S L3 |
| L5 | 1 S L4 AND ROCHER, J?/AU |
| L6 | 1 S L4 AND YAMABE, H?/AU |
| L7 | 0 S L6 NOT L5 |
| L8 | 1 S L4 AND CHAKI, H?/AU |
| L9 | 0 S L8 NOT L6 |
| L10 | 1 S L4 AND ABE, M?/AU |
| L11 | 0 S L10 NOT L6 |
| L12 | 1 S L4 AND OKUYAMA, M?/AU |
| L13 | 0 S L12 NOT L10 |

FILE 'CAOLD' ENTERED AT 15:27:42 ON 09 APR 2004

=> s 13
 L14 0 L3

| | | | |
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| => file beilstein | | | |
| COST IN U.S. DOLLARS | SINCE FILE ENTRY | TOTAL SESSION | |
| FULL ESTIMATED COST | 0.42 | 202.86 | |

| DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) | SINCE FILE ENTRY | TOTAL SESSION |
|--|------------------|---------------|
| CA SUBSCRIBER PRICE | 0.00 | -5.54 |

FILE 'BEILSTEIN' ENTERED AT 15:27:52 ON 09 APR 2004

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FILE RELOADED ON OCTOBER 20, 2002
FILE LAST UPDATED ON MARCH 30, 2004

FILE COVERS 1771 TO 2003.

FILE CONTAINS 8,932,479 SUBSTANCES

>>> PLEASE NOTE: Reaction data and substance data are stored in separate documents and can not be searched together in one query.
Reaction data for BEILSTEIN compounds may be displayed immediately with the display codes PRE (preparations) and REA (reactions). A substance answer set retrieved after the search for a chemical name, a molecular formula or a structure search for example can be restricted to compounds with available reaction information by concatenation with PRE/FA, REA/FA or more general with RX/FA. The BEILSTEIN Registry Number (BRN) is the link between a BEILSTEIN compound and belonging reactions. For more detailed reaction searches BRNs can be selected from substance answer sets and searched in the next step as reaction partner BRNs - Reactant (RX.RBRN) or Product BRN (RX.PBRN). After a search for reaction details substance documents associated with reactants or products may be retrieved by searching RX.PBRNs or RX.RBRNs as BRNs. <<<

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* ARE BASED ON THE HIGHEST PRICE CATEGORY. THEREFORE, THESE *
* ESTIMATES MAY NOT REFLECT THE ACTUAL COSTS. *
* FOR PRICE INFORMATION SEE HELP COST *

=> d his

(FILE 'HOME' ENTERED AT 15:22:35 ON 09 APR 2004)

FILE 'REGISTRY' ENTERED AT 15:22:40 ON 09 APR 2004

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| L1 | STRUCTURE UPLOADED |
| L2 | 2 S L1 |
| L3 | 45 S L1 FULL |

FILE 'HCAPLUS' ENTERED AT 15:25:39 ON 09 APR 2004

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|-----|--------------------------|
| L4 | 7 S L3 |
| L5 | 1 S L4 AND ROCHER, J?/AU |
| L6 | 1 S L4 AND YAMABE, H?/AU |
| L7 | 0 S L6 NOT L5 |
| L8 | 1 S L4 AND CHAKI, H?/AU |
| L9 | 0 S L8 NOT L6 |
| L10 | 1 S L4 AND ABE, M?/AU |

L11 0 S L10 NOT L6
 L12 1 S L4 AND OKUYAMA, M?/AU
 L13 0 S L12 NOT L10

FILE 'CAOLD' ENTERED AT 15:27:42 ON 09 APR 2004
 L14 0 S L3

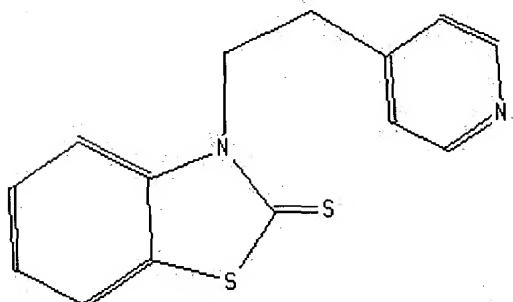
FILE 'BEILSTEIN' ENTERED AT 15:27:52 ON 09 APR 2004

=> s 13
 L15 1 L3

=> d 115

L15 ANSWER 1 OF 1 BEILSTEIN COPYRIGHT 2004 BEILSTEIN MDL on STN

| | |
|----------------------------|--|
| Beilstein Records (BRN) : | 1217129 |
| Beilstein Pref. RN (BPR) : | <u>27410-87-3</u> |
| CAS Reg. No. (RN) : | 27410-87-3 |
| Chemical Name (CN) : | 3-(2-pyridin-4-yl-ethyl)-3H-benzothiazole-2-thione |
| Autonom Name (AUN) : | 3-(2-pyridin-4-yl-ethyl)-3H-benzothiazole-2-thione |
| Molec. Formula (MF) : | C14 H12 N2 S2 |
| Molecular Weight (MW) : | 272.38 |
| Lawson Number (LN) : | 31156, 27396 |
| Compound Type (CTYPE) : | heterocyclic |
| Constitution ID (CONSID) : | 1157666 |
| Tautomer ID (TAUTID) : | 1192884 |
| Beilstein Citation (BSO) : | 5-27, 6-27 |
| Entry Date (DED) : | 1988/11/29 |
| Update Date (DUPD) : | 1993/02/15 |



Field Availability:

| Code | Name | Occurrence |
|-------|------------------------|------------|
| <hr/> | | |
| BRN | Beilstein Records | 1 |
| BPR | Beilstein Preferred RN | 1 |
| RN | CAS Registry Number | 1 |
| CN | Chemical Name | 1 |
| AUN | Autonomname | 1 |
| MF | Molecular Formula | 1 |
| FW | Formular Weight | 1 |
| LN | Lawson Number | 2 |

| | | |
|--------|----------------------------|---|
| CTYPE | Compound Type | 1 |
| CONSID | Constitution ID | 1 |
| TAUTID | Tautomer ID | 1 |
| BSO | Beilstein Citation | 2 |
| ED | Entry Date | 1 |
| UPD | Update Date | 1 |
| IR | Infrared Spectrum | 2 |
| MP | Melting Point | 4 |
| MS | Mass Spectrum | 1 |
| NMR | Nuclear Magnetic Resonance | 4 |
| UVS | UV and Visible Spectrum | 1 |

This substance also occurs in Reaction Documents:

| Code | Name | Occurrence |
|-------|-------------------------------|------------|
| <hr/> | | |
| RX | Reaction Documents | 3 |
| RXPRO | Substance is Reaction Product | 3 |

=> fil reg; d acc 27410-87-3; fil BEILSTEIN

FILE 'REGISTRY' ENTERED AT 15:28:21 ON 09 APR 2004

ANSWER 1 REGISTRY COPYRIGHT 2004 ACS on STN

RN 27410-87-3 REGISTRY

CN 2 (3H)-Benzothiazolethione, 3-[2-(4-pyridinyl)ethyl]- (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

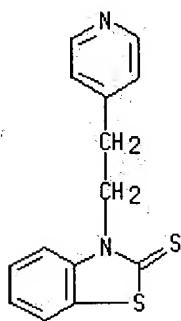
CN 2-Benzothiazolinethione, 3-[2-(4-pyridyl)ethyl]- (8CI)

FS 3D CONCORD

MF C14 H12 N2 S2

LC STN Files: BEILSTEIN*, CA, CAPLUS, CASREACT, CHEMCATS, IFICDB, IFIPAT, IFIUDB

(*File contains numerically searchable property data)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

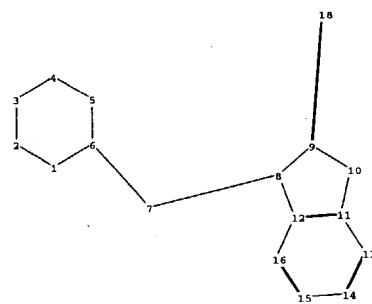
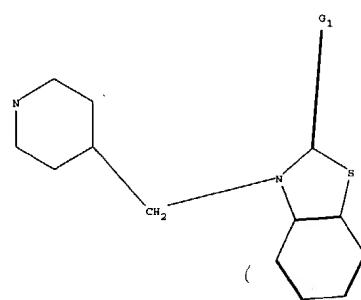
3 REFERENCES IN FILE CA (1907 TO DATE)

3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

FILE 'BEILSTEIN' ENTERED AT 15:28:21 ON 09 APR 2004

| | | | |
|--|------------------|---------------|--|
| => log Y | | | |
| COST IN U.S. DOLLARS | SINCE FILE ENTRY | TOTAL SESSION | |
| FULL ESTIMATED COST | 0.06 | 215.28 | |
| DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) | SINCE FILE ENTRY | TOTAL SESSION | |
| CA SUBSCRIBER PRICE | 0.00 | -5.54 | |

STN INTERNATIONAL LOGOFF AT 15:28:27 ON 09 APR 2004



chain nodes :

7 18

ring nodes :

1 2 3 4 5 6 8 9 10 11 12 13 14 15 16

chain bonds :

6-7 7-8 9-18

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 8-9 8-12 9-10 10-11 11-12 11-13 12-16 13-14 14-15
15-16

exact/norm bonds :

1-2 1-6 2-3 3-4 4-5 5-6 8-9 8-12 9-18

exact bonds :

6-7 7-8 9-10 10-11

normalized bonds :

11-12 11-13 12-16 13-14 14-15 15-16

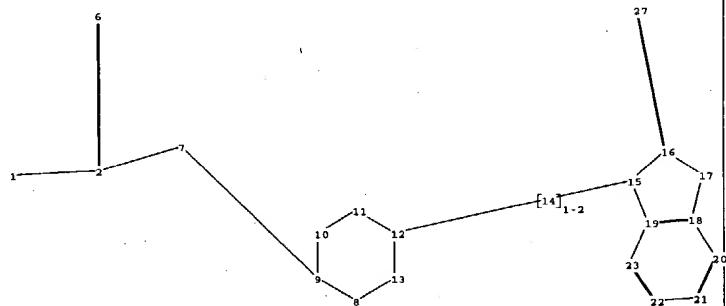
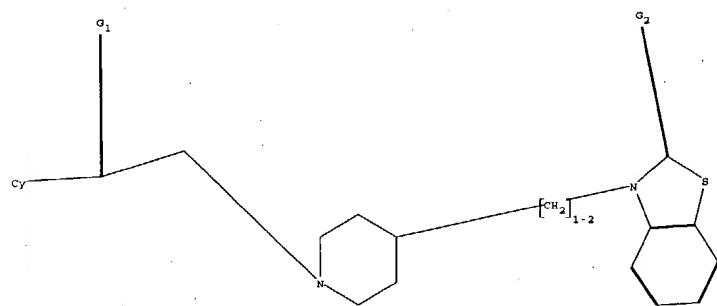
isolated ring systems :

containing 1 : 8 :

G1:O,S

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:Atom 9:Atom 10:Atom 11:Atom
12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 18:CLASS

¹
N¹
O

chain nodes :

1 2 3 6 7 14 27

ring nodes :

8 9 10 11 12 13 15 16 17 18 19 20 21 22 23

chain bonds :

1-2 2-6 2-7 7-9 12-14 14-15 16-27

ring bonds :

8-9 8-13 9-10 10-11 11-12 12-13 15-16 15-19 16-17 17-18 18-19 18-20 19-23
20-21 21-22 22-23

exact/norm bonds :

1-2 2-6 7-9 8-9 8-13 9-10 10-11 11-12 12-13 15-16 15-19 16-27

exact bonds :

2-7 12-14 14-15 16-17 17-18

normalized bonds :

18-19 18-20 19-23 20-21 21-22 22-23

isolated ring systems :

containing 8 : 15 :

G1:0,[*1]

G2:0,S

Match level :

1:Atom 2:CLASS 3:CLASS 6:CLASS 7:CLASS 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom
13:Atom 14:CLASS 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom 22:Atom
23:Atom 27:CLASS

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| <u>NEWS 3</u> | NOV 24 MSDS-CCOHS file reloaded |
| <u>NEWS 4</u> | DEC 08 CABA reloaded with left truncation |
| <u>NEWS 5</u> | DEC 08 IMS file names changed |
| <u>NEWS 6</u> | DEC 17 DGENE: Two new display fields added |
| <u>NEWS 7</u> | DEC 18 BIOTECHNO no longer updated |
| <u>NEWS 8</u> | DEC 19 CROPUS no longer updated; subscriber discount no longer available |
| <u>NEWS 9</u> | DEC 22 ABI-INFORM now available on STN |
| <u>NEWS 10</u> | JAN 27 Source of Registration (SR) information in REGISTRY updated and searchable |
| <u>NEWS 11</u> | JAN 27 A new search aid, the Company Name Thesaurus, available in CA/CAplus |
| <u>NEWS 12</u> | FEB 05 German (DE) application and patent publication number format changes |
| <u>NEWS 13</u> | MAR 03 MEDLINE and LMEDLINE reloaded |
| <u>NEWS 14</u> | MAR 03 MEDLINE file segment of TOXCENTER reloaded |
| <u>NEWS 15</u> | MAR 03 FRANCEPAT now available on STN |
| <u>NEWS 16</u> | MAR 29 Pharmaceutical Substances (PS) now available on STN |
| <u>NEWS 17</u> | MAR 29 WPIVF now available on STN |
| <u>NEWS 18</u> | MAR 29 No connect hour charges in WPIVF until May 1, 2004 |
| <u>NEWS 19</u> | MAR 29 New monthly current-awareness alert (SDI) frequency in RAPRA |
| <u>NEWS EXPRESS</u> | MARCH 31 CURRENT WINDOWS VERSION IS V7.00A, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 3 MARCH 2004 |
| <u>NEWS HOURS</u> | STN Operating Hours Plus Help Desk Availability |
| <u>NEWS INTER</u> | General Internet Information |
| <u>NEWS LOGIN</u> | Welcome Banner and News Items |
| <u>NEWS PHONE</u> | Direct Dial and Telecommunication Network Access to STN |
| <u>NEWS WWW</u> | CAS World Wide Web Site (general information) |

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* * * * * * * * * * STN Columbus * * * * * * * * * * *

FILE 'HOME' ENTERED AT 14:11:42 ON 09 APR 2004

| => file reg | SINCE FILE ENTRY | TOTAL SESSION |
|----------------------|------------------|---------------|
| COST IN U.S. DOLLARS | | |
| FULL ESTIMATED COST | 0.21 | 0.21 |

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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 7 APR 2004 HIGHEST RN 672883-15-7
 DICTIONARY FILE UPDATES: 7 APR 2004 HIGHEST RN 672883-15-7

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:
<http://www.cas.org/ONLINE/DBSS/registryss.html>

```
=>
L1      STRUCTURE UPLOADED

=> d 11
L1 HAS NO ANSWERS
L1      STR

=> s 11
SAMPLE SEARCH INITIATED 14:13:31 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -      2 TO ITERATE

100.0% PROCESSED      2 ITERATIONS          1 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:      2 TO      124
PROJECTED ANSWERS:         1 TO      80
```

L2 1 SEA SSS SAM L1

```
=> s 11 full
THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 155.00 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
FULL SEARCH INITIATED 14:13:35 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -      44 TO ITERATE
```

```
100.0% PROCESSED      44 ITERATIONS        18 ANSWERS
SEARCH TIME: 00.00.01
```

L3 18 SEA SSS FUL L1

| | | |
|----------------------|------------|---------|
| => file hcaplus | SINCE FILE | TOTAL |
| COST IN U.S. DOLLARS | ENTRY | SESSION |
| FULL ESTIMATED COST | 156.26 | 156.47 |

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FILE COVERS 1907 - 9 Apr 2004 VOL 140 ISS 16
FILE LAST UPDATED: 8 Apr 2004 (20040408/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s 13
L4 1 L3

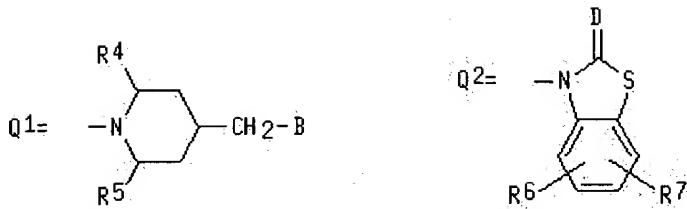
=> d 14, ibib abs fhitstr, 1

L4 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Citing
 Text References

ACCESSION NUMBER: 1999:311193 HCAPLUS
DOCUMENT NUMBER: 130:338102
TITLE: Preparation of N-(aminoalkyl)- or N-(1-piperidinylmethyl)benzothiazoline derivatives as ligands for sigma-receptor
INVENTOR(S): Rocher, Jean-Philippe; Yamabe, Haruko; Chaki, Haruyuki; Saito, Ken-ichi; Abe, Michikazu; Okuyama, Masahiro
PATENT ASSIGNEE(S): Mitsubishi Chemical Corporation, Japan
SOURCE: PCT Int. Appl., 95 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|--|--------|------------|-----------------|------------|
| WO 9923083 | A1 | 19990514 | WO 1998-JP4973 | 19981104 |
| W: CA, CN, KR, US | | | | |
| RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE | | | | |
| EP 1043319 | A1 | 20001011 | EP 1998-951687 | 19981104 |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI | | | | |
| JP 11217377 | A2 | 19990810 | JP 1998-314459 | 19981105 |
| PRIORITY APPLN. INFO.: | | | JP 1997-302607 | A 19971105 |
| | | | WO 1998-JP4973 | W 19981104 |
| OTHER SOURCE(S): | MARPAT | 130:338102 | | |
| GI | | | | |



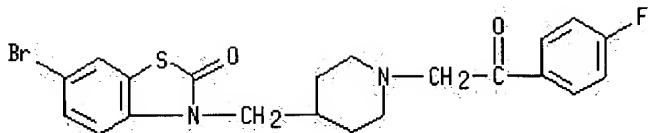
AB Compds. represented by the following formula, such as (R,S)-1-(1-adamantyl)-2-[4-(6-chloro-2-iminobenzothiazolin-3-ylmethyl)piperidin-1-yl]ethanol, or salts thereof: X-Q-C(R1)(R2)-Z [wherein R1 and R2 each represents hydrogen, alkyl, cycloalkyl, hydroxyalkyl, or alkenyl; and Z represents either of groups NR₃(CH₂)_p and Q1; wherein R₃ represents alkyl, cycloalkyl, hydroxyalkyl, or alkenyl; p is an integer of 3 to 8; R₄ and R₅ each represents hydrogen or alkyl or they together with other interposing atoms represent a 5- to 7-membered heterocyclic ring; and B represents formula Q2 (wherein R₆ and R₇ each represents hydrogen, halogeno, NO₂, alkyl, cycloalkyl, alkenyl, haloalkyl, OH, alkoxy, haloalkoxy, alkoxy carbonyl, Ph, (un)substituted NH₂, alkylthio, etc.); D represents sulfur, oxygen, or (un)substituted NH; when X represents optionally alkyl-substituted mono- or polycyclic alkyl, cycloalkylalkyl, aryl, or heteroaryl, Q represents CO, C(:NOH), C(Y)(A) (wherein Y represents H, alkyl, alkenyl, alkynyl, etc. and A represent OH, alkoxy, cycloalkoxy, cycloalkylalkoxy, alkenyloxy, aryloxy, etc.); or when X represents a 8- to 10-membered bicyclic heteroaryl contg. 1 or 2 heteroatoms, Q represents single bond], which have high affinity to σ -receptors and exhibit small inhibition consts. Ki against σ -1 and/or σ -2 receptors, are prep'd. Also claimed are therapeutics contg. I as the active ingredients for the treatment and/or prevention of diseases caused or enhanced by nerve-regulating effect of σ -ligands. They are useful for the treatment and/or prevention of central nervous system diseases, intestinal diseases, and cardiovascular diseases. Thus, 4-(6-chloro-2-iminobenzothiazolin-3-ylmethyl)piperidine was condensed with 1-(bromoacetyl)adamantane in the presence of K₂CO₃ followed by NaBH₄ redn. in ethanol and THF and acidification with HCl in EtOAc to give 1-(1-adamantyl)-2-[4-(6-chloro-2-iminobenzothiazolin-3-ylmethyl)piperidin-1-yl]ethanol hydrochloride (II). II and 3-[[1-[2-(4-fluorophenyl)-2-oxoethyl]-4-piperidinyl]methyl]-5-chloro-2-oxobenzothiazoline hydrochloride inhibited the binding of [H₃]-di-o-tolylguanidine to σ -receptor (P2 membrane fraction) prep'n. from rat liver with Ki value of 7.0 and 3.1 nM, resp., as compared to Ki of 29 nM for haloperidol. A tablet, an injection, and an ointment formulation contg. II were described.

IT 224443-05-4P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prep'n. of N-(aminoalkyl)- or N-(1-piperidinyl)benzothiazoline derivs.
having high affinity to sigma-receptor as therapeutics)

RN 224443-05-4 HCPLUS

CN 2(3H)-Benzothiazolone, 6-bromo-3-[[1-[2-(4-fluorophenyl)-2-oxoethyl]-4-piperidinyl]methyl]-, monohydrochloride (9CI) (CA INDEX NAME)



HC1

REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> file caold
COST IN U.S. DOLLARS

| SINCE FILE ENTRY | TOTAL SESSION |
|------------------|---------------|
| 7.12 | 163.59 |

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

| SINCE FILE ENTRY | TOTAL SESSION |
|------------------|---------------|
| -0.69 | -0.69 |

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FILE COVERS 1907-1966

FILE LAST UPDATED: 01 May 1997 (19970501/UP)

This file contains CAS Registry Numbers for easy and accurate substance identification. Title keywords, authors, patent assignees, and patent information, e.g., patent numbers, are now searchable from 1907-1966. TIFF images of CA abstracts printed between 1907-1966 are available in the PAGE display formats.

This file supports REGISTRY for direct browsing and searching of all substance data from the REGISTRY file. Enter HELP FIRST for more information.

=> d his

(FILE 'HOME' ENTERED AT 14:11:42 ON 09 APR 2004)

FILE 'REGISTRY' ENTERED AT 14:11:48 ON 09 APR 2004

| | |
|----|--------------------|
| L1 | STRUCTURE UPLOADED |
| L2 | 1 S L1 |
| L3 | 18 S L1 FULL |

FILE 'HCAPLUS' ENTERED AT 14:13:38 ON 09 APR 2004

| | |
|----|--------|
| L4 | 1 S L3 |
|----|--------|

FILE 'CAOLD' ENTERED AT 14:13:48 ON 09 APR 2004

=> s 13
L5 0 L3

=> file beilstein
COST IN U.S. DOLLARS SINCE FILE TOTAL

| | ENTRY | SESSION |
|--|------------|---------|
| FULL ESTIMATED COST | 0.42 | 164.01 |
| DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) | SINCE FILE | TOTAL |
| CA SUBSCRIBER PRICE | ENTRY | SESSION |
| | 0.00 | -0.69 |

FILE 'BEILSTEIN' ENTERED AT 14:13:56 ON 09 APR 2004

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FILE RELOADED ON OCTOBER 20, 2002
FILE LAST UPDATED ON MARCH 30, 2004

FILE COVERS 1771 TO 2003.

FILE CONTAINS 8,932,479 SUBSTANCES

>>> PLEASE NOTE: Reaction data and substance data are stored in separate documents and can not be searched together in one query.

Reaction data for BEILSTEIN compounds may be displayed immediately with the display codes PRE (preparations) and REA (reactions). A substance answer set retrieved after the search for a chemical name, a molecular formula or a structure search for example can be restricted to compounds with available reaction information by concatenation with PRE/FA, REA/FA or more general with RX/FA. The BEILSTEIN Registry Number (BRN) is the link between a BEILSTEIN compound and belonging reactions. For more detailed reaction searches BRNs can be selected from substance answer sets and searched in the next step as reaction partner BRNs - Reactant (RX.RBRN) or Product BRN (RX.PBRN). After a search for reaction details substance documents associated with reactants or products may be retrieved by searching RX.PBRNs or RX.RBRNs as BRNs. <<<

>>> FOR SEARCHING PREPARATIONS SEE HELP PRE <<<

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* SET NOTICE FEATURE: THE COST ESTIMATES CALCULATED FOR SET NOTICE *
* ARE BASED ON THE HIGHEST PRICE CATEGORY. THEREFORE; THESE *
* ESTIMATES MAY NOT REFLECT THE ACTUAL COSTS. *
* FOR PRICE INFORMATION SEE HELP COST *

=> s 13
L6 0 L3

| | | |
|--|------------|---------|
| COST IN U.S. DOLLARS | SINCE FILE | TOTAL |
| FULL ESTIMATED COST | ENTRY | SESSION |
| 0.42 | 164.43 | |
| DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) | SINCE FILE | TOTAL |
| CA SUBSCRIBER PRICE | ENTRY | SESSION |
| 0.00 | -0.69 | |

STN INTERNATIONAL LOGOFF AT 14:14:06 ON 09 APR 2004

